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AUTHOR(S): P.-M. Binder

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STATISTICAL PROPERTIES OF LORENTZ LATTICE GASES

P.-M. Binder

Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545

and

Applied Physics Section, Yale University, New Haven, CT 06520

In this paper we present new results for the long-time tails and mean-square displacement evolution for several deterministic and probabilistic models of the Lorentz gas in a square lattice. The simulations give diffusion coefficients which agree with analytical results from the corresponding Boltzmann equation. For long times, abnormal diffusion is observed for the deterministic models only. This is probably due to recurring trajectories. The velocity autocorrelation function shows exponents which vary between -1 and -2 depending on the particle-scatterer collision model used.

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1. Introduction

This paper contains new results, mostly numerical, on the diffusion and long-time tails of several lattice models of the Lorentz gas. These models are very similar to those I presented in a previous paper[1], although here I will treat both deterministic and probabilistic collision models in a square lattice only. These models are loosely based on recent developments in lattice gases[2,3]. The main features of these models are that time and space are discrete, and that particles and scatterers occupy no volume.

My results are as follows. (1) Numerical simulations for the mean-square displacement (m.s.d), $< \Delta r^2 >$ versus time, yield diffusion coefficients which agree well with analytical results at the Boltzmann level (low-density) up to scatterer concentrations of 0.3. (2) For the deterministic collision models only, the m.s.d. becomes constant after long times, of the order of several hunded mean-free paths. We present numerical evidence to link this result to recurring trajectories. (3) I present results for the velocity autocorrelation function, $C(t) = < v(0)v(t) >$. This quantity exhibits a power- law decay (long-time tails) with the power varying between -1 for deterministic rules and -2 for random, uniform scattering. These results are valid for just a few mean-free paths, before statistical noise takes over.

In the remainder of this section I will introduce the Lorentz model, and a few basic results. In section 2 I will review recent work on lattice models with static disorder, including the models studied in this paper. In sections 3 and 4 I present the results for diffusive behavior and long-time tails respectively. A discussion in section 5 concludes this paper.

The Lorentz gas, in which a single particle moves through an array of randomly placed fixed disk scatterers[4] was originally proposed by Lorentz as a model of electron motion in a solid. It has turned out to be, along with Ehrenfest's wind-tree model[5], a similar model with diamond-shaped scatterers, an important test case in kinetic theory. For one thing, the low-density description is given by a linear Boltzmann equation, which has allowed for explicit analytical solutions. See, for example, Reference (6) for a review. Also, the high-density diffusion coefficient has been worked out, at least for the wind-tree model[7]. Another aspect of interest in this problem is the C(t) function defined above. It has been shown by momentum conservation arguments[8] that this quantity should go as $t^{d/2}$ for d-dimensional gases. The Lorentz gas does not conserve momentum, and Ernst and Weyland[9] showed that for this gas $C(t) \sim t^{-(d+1)/2}$. There is strong disagreement in two dimensions between this result and computer simulations[10]. Although at least two possible explanations have been proposed, one in terms of slow convergence to asymptotic behavior[11] and the other in terms of a crossover near the percolation density of scatterers[12], this is still an open problem. I will now review recent work on Lorentz-like models in lattices.

2. The Lorentz gas: lattice models

This section begins with two warnings: the survey may not be complete, and there will be a lot of emphasis on my own models- mainly because the results in the following two sections are based on these models.

Gates and others[13-15] have studied certain properties of wind-tree models in a lattice. Each scatterer effectively occupies four lattice sites. In References (13-14), Gates proved some existence theorems for the diffusion coefficient in these models. One of the models in Reference (14), proposed by Kac, is very similar to my models (it has point scatterers), except that his particles always turn in the same direction. Reference (15) models a kind of multiple collision studied earlier in Reference (7), by placing parallel mirrors in a lattice.

In a paper mostly about one-dimensional stochastic Lorentz gases, van Beijeren[8] suggests two-dimensional stochastic Lorentz gases on a lattice which are a generalization of some of the models I study in the next two sections. Apparently, no results existed at the time for these models. Finally, Ernst and others[11,12] have studied hopping models in a lattice with random excluded sites. Although this problem differs a lot from the Lorentz gas (for example, the concept of mean-free path makes no sense), it still has the effect of static disordered structures affecting particle motion. These papers present very interesting results, especially for the velocity autocorrelation function. I will now explain the models in Reference (1), along with some basic results, as well as the models studied in the present paper.

Three models were proposed in that paper. We will call them square lattice (S), triangular, time-alternating (TTA) and triangular, time-independent (TTI). The models in the present paper are all variations on (S). These models have two common features: they are discrete in time and they are formulated in a regular plane-filling lattice (square or triangular). For simplicity, we will take the edge length, time step and velocity of the particle to be equal to one, so that all distributions, diffusion coefficients and recurrence times come out dimensionless. Note that with this simplification the mean free time and the mean free path are the same. In the first model, the particle moves between the nodes of a square grid at unit speed. The direction of the particle only changes when it hits a scatterer (randomly placed at the nodes of the grid). It does so by $\pm 90^0$, according to the parity of the time step.

In the other two models, the particle moves in a triangular grid, so that at each node 6 directions – differing by factors of 60^0– are possible. Unless a scatterer is present, the particle will go through a node without change in velocity. In the TTA case, the particle will undergo a $\pm 60^0$ change in direction, according to the parity of the time step. In the TTI case, a scatterer will always cause a 60^0 deviation in the same direction, so, after 6 collisions, the particle will have traveled in every possible direction.

In all models I used a parallelogram-shaped domain with helical boundary conditions, to ensure that in the absence of scatterers the particle would show some semblance of ergodic behavior. A typical trajectory, obtained in a CAM-6 machine[16] appears in Figure 1.

I studied three physical properties of these models: (a) the dependence of mean free path on the density of scatterers, which agrees with analytical results[17]; (b) the long-time displacement distribution, which is consistent with analytical results[18], and (c) the diffusion coefficient. Although the time dependence of the mean-square displacement shows that this coefficient is well defined, at least for short times, its dependence on density of scatterers disagrees somewhat with analytical results for the Ehrehfest wind-tree model. This is to be expected from the nature of our model, which does not restrict particle motion at high density of scatterers.

I also studied the state-transition graphs of the gas viewed as a discrete dynamical system: these graphs share to a large extent the properties of chaotic[19] and random[20] discrete maps for the distribution of limit cycles :

(a) Starting from an initial condition picked at random, there is a uniform probability distribution for the length of cycles.

(b) The average length of a cycle that starts from an initial condition picked at random is $\frac{m}{2}$, where m is the total number of states.

(c) The average number of cycles is equal to $ln(m)$.

For the Lorentz gas we see that the property (b) holds for all models, property (a) holds fairly well (especially for the TTI model), and property (c) is in fair agreement with the behavior of a chaotic map, and at high scatterer densities agrees well with the result for a random mapping. Although somewhat indirect, these results are consistent with the analytical and numerical results that the Lorentz gas exhibits chaotic behavior [21].

In the present paper the (S) model will be called the "deteministic" model, and a version of (S) in which the direction of motion changes at random rather than by the parity of the time step will be called "probabilistic".

3. Diffusive behavior

This section contains results of simulations of both the deterministic and probabilistic models. The scatterers were generated along the trajectory of a single particle with probability c (c=concentration), keeping track of previously visited sites. Only trajectories which after 5000 time steps had a number of scatterers agreeing within 5% with the density were kept for averaging. Figure 2 shows the m.s.d., $< (r(0) - r(t))^2 >$ versus time for (a) the deterministic model and (b) the probabilistic model, for c=0.3. From this plot, the diffusion coefficient can be computed by Einstein's equation[22],

$$< \Delta r^2 > = 4Dt \qquad (1)$$

Figure 3 shows the numerical values of D for $0.05 < c < 0.3$, which compare well with analytical results for the Boltzmann equation. At low densities, for both the deterministic and probabilistic models, the distribution of particles is governed by

$$f_i(n+\rho_i, t+1) = (1-c) f_i(n,t) + \frac{c}{2}[f_{i-1}(n,t) + f_{i+1}(n,t)] \qquad 2$$

where f_j is the distribution of particles moving with velocity j (the cyclic index j varies between 0 and 3; for example, 0 is the +x direction), n is a node label, ρ_i is a unit vector in direction i and c is the concentration. Upon substituting the mode expressions

$$f_j = A_j e^{i(q \cdot \rho_j - \omega(t))} \qquad 3$$

one gets four equations for the amplitudes A_j. After linearizing and solving for the eigenvalues, one gets

$$\omega = \frac{1}{2c} q^2 = D q^2 \qquad 4$$

which is the straight line in Figure 3. A complete derivation for arbitrary collision rules, of which the ones here are a special case, will be presented elsewhere.

The most striking difference between Figures 2(a) and 2(b) is the fact that $< \Delta r^2 >$ stays at a constant value for long enough times. This appears to be caused by limit cycles in the particle trajectory. These cycles are only possible in the deterministic model. The simplest configuration of scatterers that could support such a trajectory is four scatterers at the vertices of a 2x2 square. I plan to use distributions of these limit cycles, such as Figure 4, to explain the time it takes for this phenomenon to appear and the final value of $< \Delta r^2 >$. This is an extreme case of the abnormal diffusion studied in [7], and was first predicted by J.Machta[23].

4. Velocity autocorrelation functions

The simulations here are very similar to those in the previous section, except that they involve more configurations of scatterers (up to 100,000 as opposed to 5,000 for the diffusion coefficient) and fewer time steps (up to 100).

Figure 5 shows C(t) for c=0.3 for (a) the deterministic model and (b) the probabilistic model. Note that in the deterministic model the curve reflects the influence of the parity of the time step, which is not the case in the probabilistic model. Figure 6 shows log C(t) versus log t for the deterministic and probabilistic models, the upper and lower curves respectively (c=0.2). After about 50 time steps, the statistical error becomes very large. The fact that the correlation decays more slowly for the deterministic model is to be expected. The exponents are independent of density, and appear to be -1 for the deterministic case and about -1.7 for the probabilistic one. A similar curve for random, uniform scattering at c=0.1 is shown in Figure 7. This is the only one which agrees with the prediction $C(t) \sim t^{-2}$. I have at the present no analytical results for these models.

5. Discussion

This paper presents several new results for lattice models of the Lorentz gas. It extends the diffusion calculations of Reference (1) from 20 mean- free paths to a few hundred. It introduces probabilistic models in addition to deterministic ones, and shows important differences in their behavior for long times. What we observe in the deterministic model is an extreme case of the abnormal difusion studied in Reference (7). This is caused by recurring trajectories, which are an infinite limit of orbiting events. I show that the recurring events are very common for this model. I also present the Boltzmann-level results for these models, which indeed show agreement at low density of scatterers. Finally, I show numerical results for the velocity autocorrelation function. A power law decay is indeed obeyed, but only one of the models agrees with the theoretical exponent. Two surprising results are the density independence and the model dependence of this exponent.

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Figure Titles

1. Recurring trajectories in a 252X251 lattice, TTA model, with reflecting boundary conditions: 25% scatterers (length: 85089);

2. Mean-square displacement versus time: (a) deterministic model, (b) probabilistic model, for c=0.3.

3. Logarithm of the diffusion coefficient vs. logarithm of the density. Straight line: Boltzmann equation results; circles: deterministic model; squares: probabilistic model.

4. Distribution of limit cycle lengths for c=0.1.

5. C(t) for (a) deterministic model, (b) probabilistic model, c=0.3

6. Logarithm of C(t) versus log t. The slope of this curve giv the exponent of the long-time tails. Upper curve: deterministic model, lower curve: probabilistic model. Scatterer density=0.2.

7. Logarithm of C(t) versus log t for random, uniform scattering. Scatterer density=0.1.

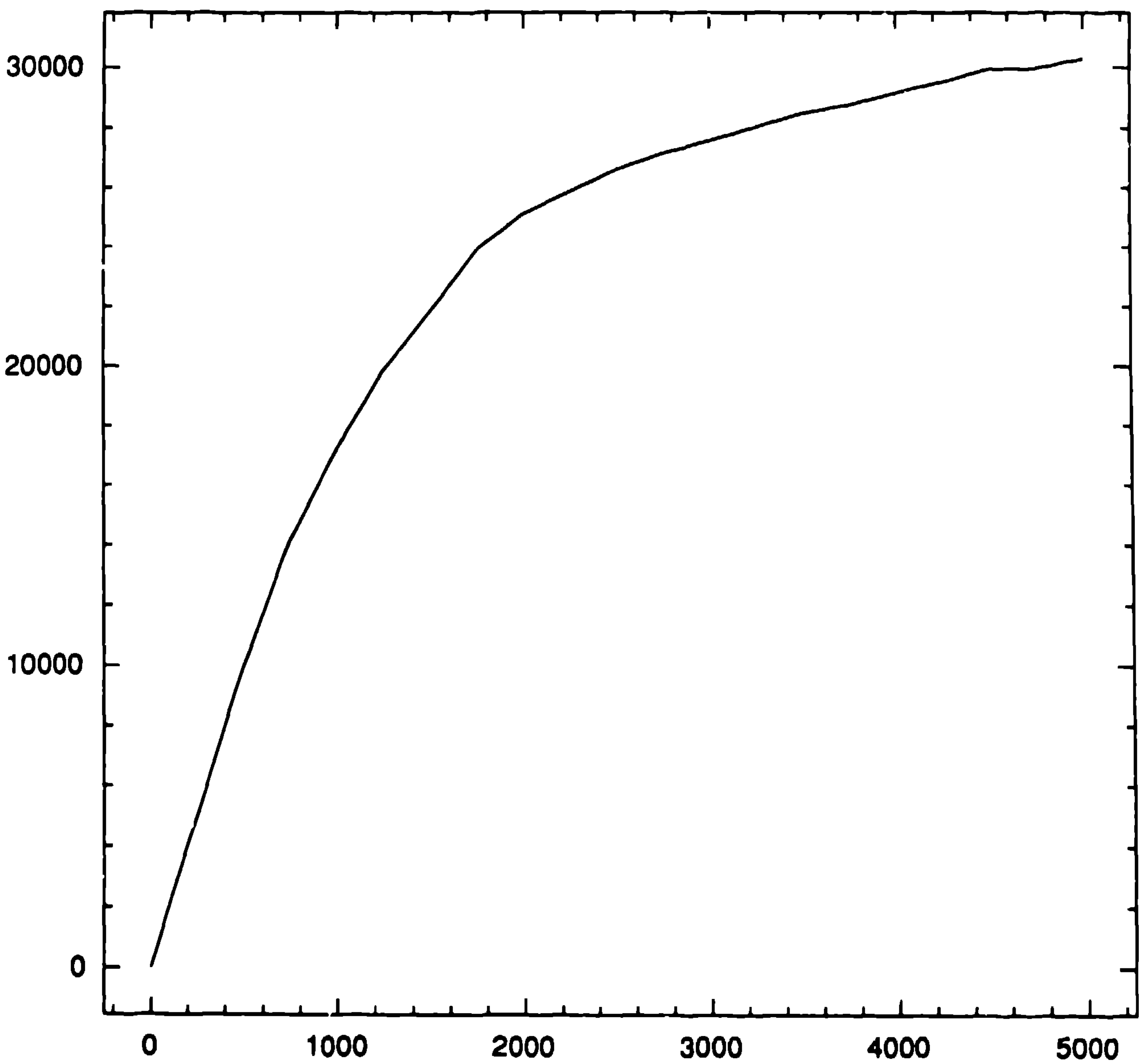


Figure 2(a)

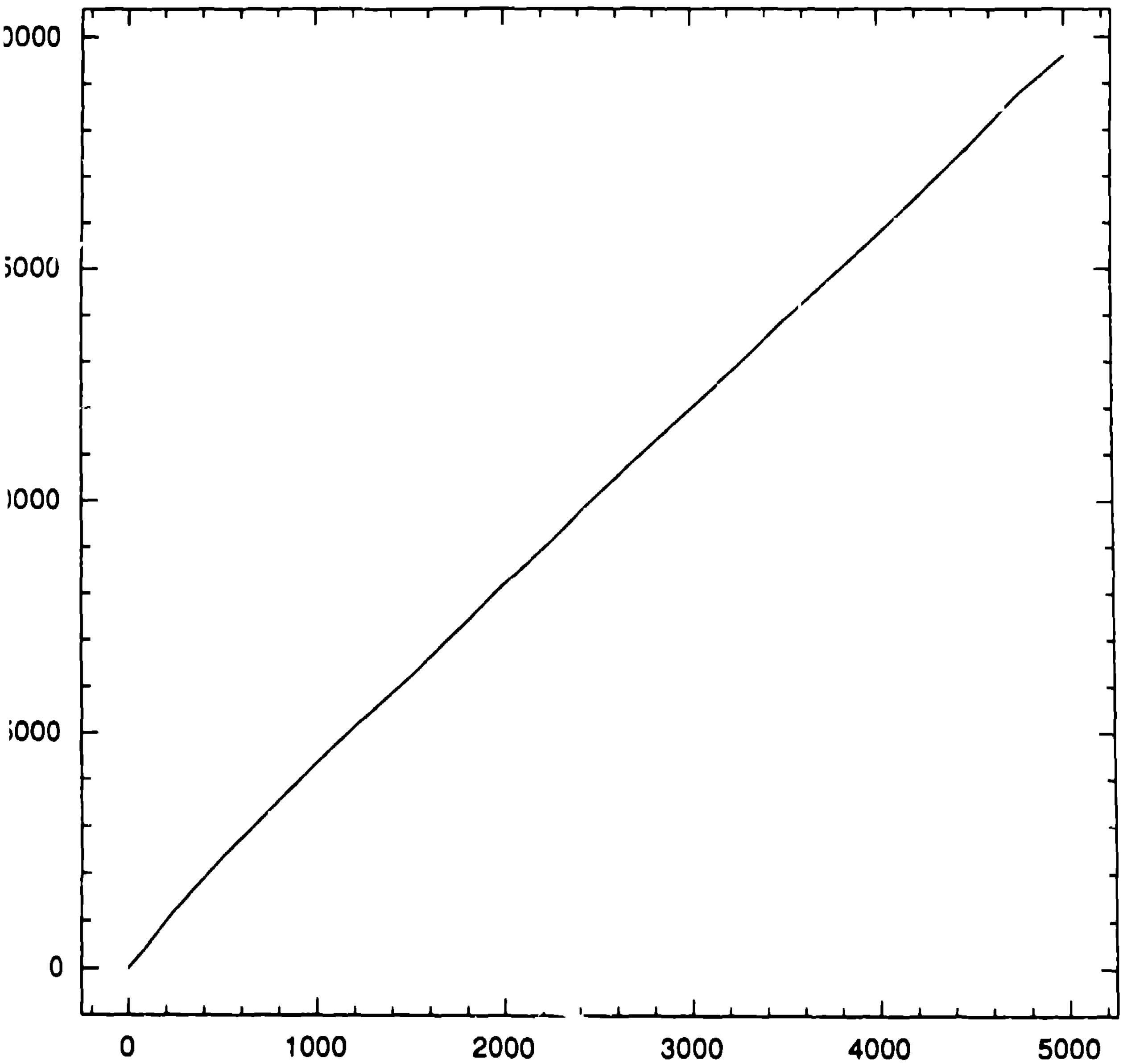
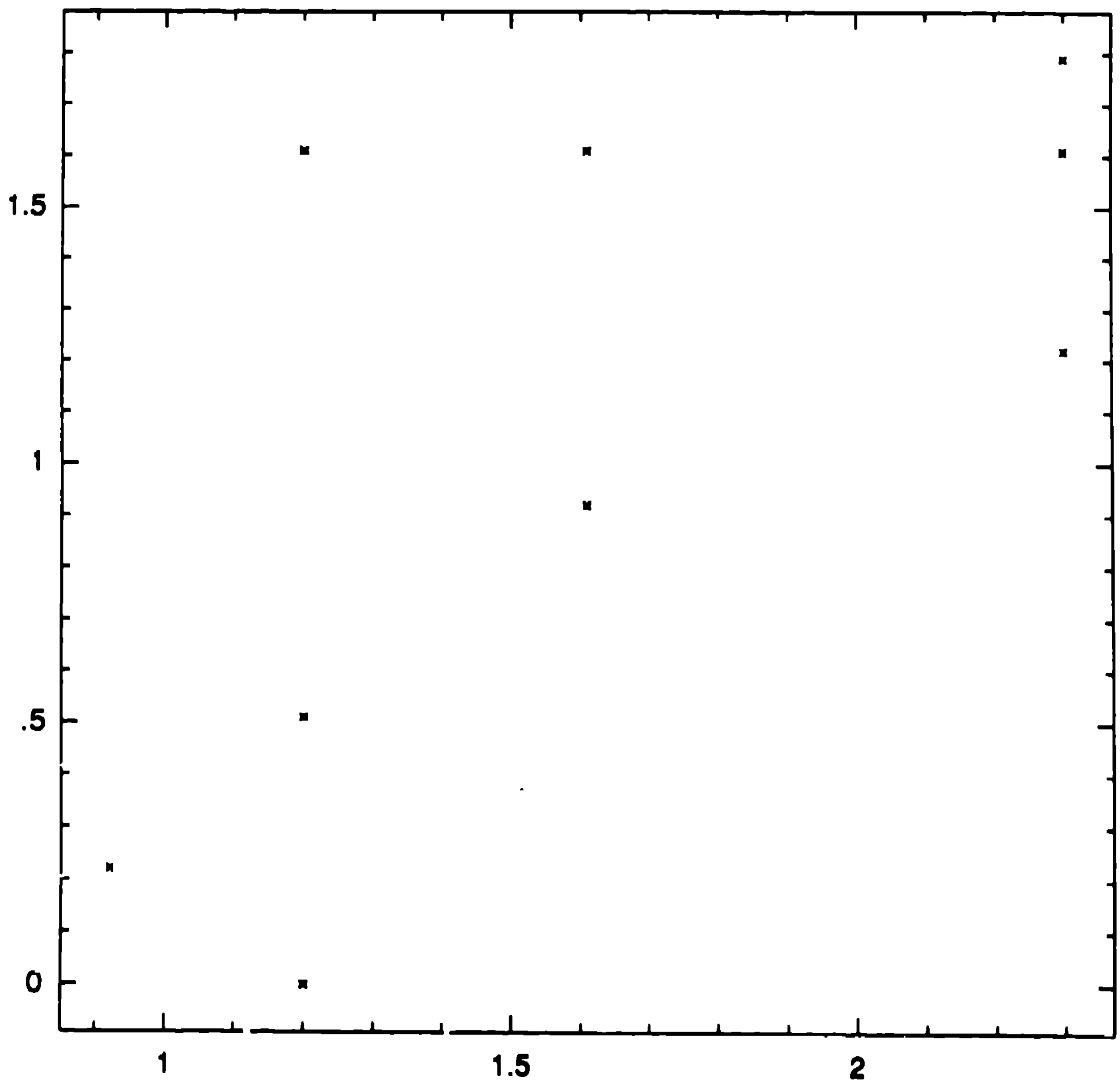


Figure 2(c)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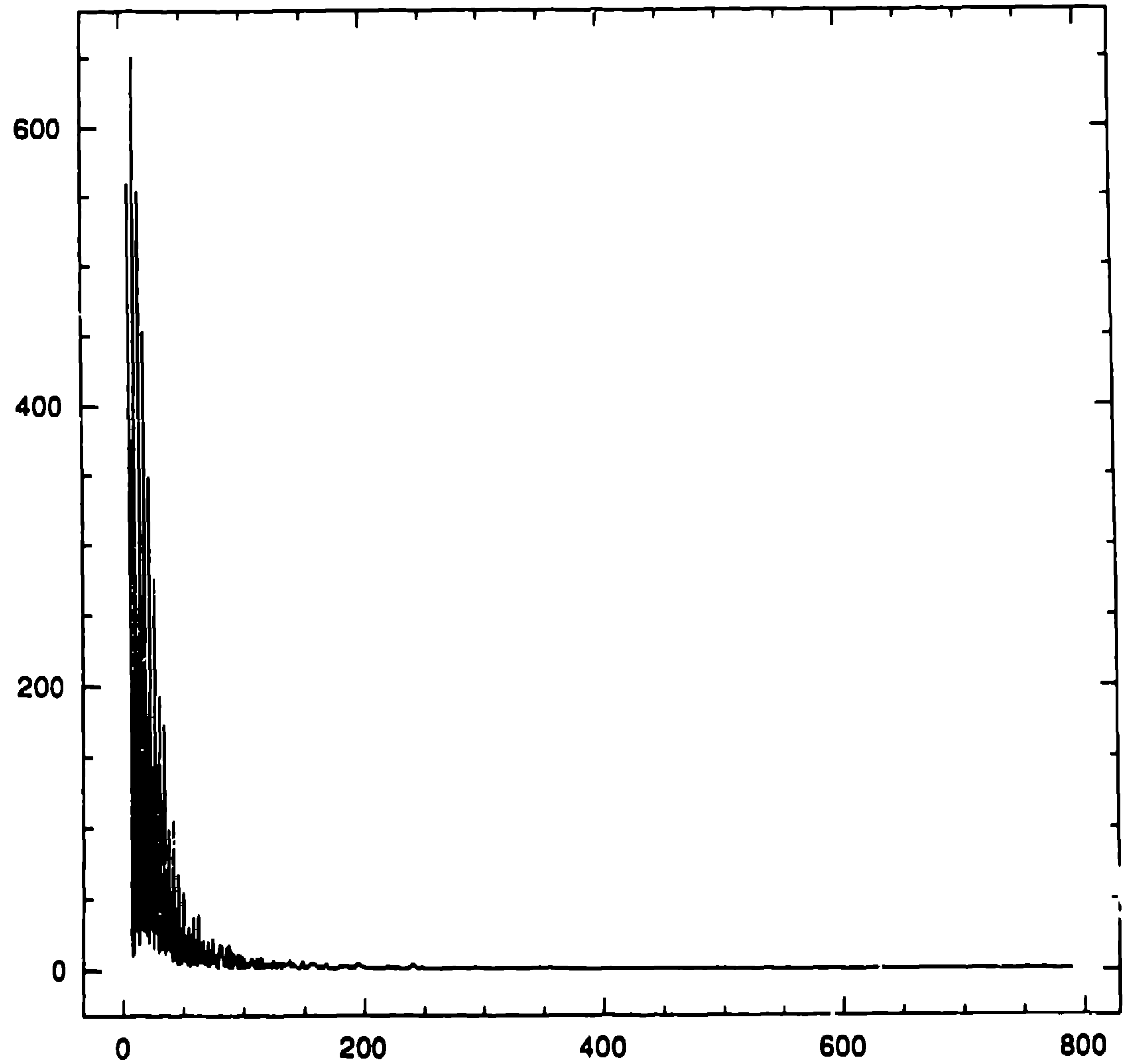

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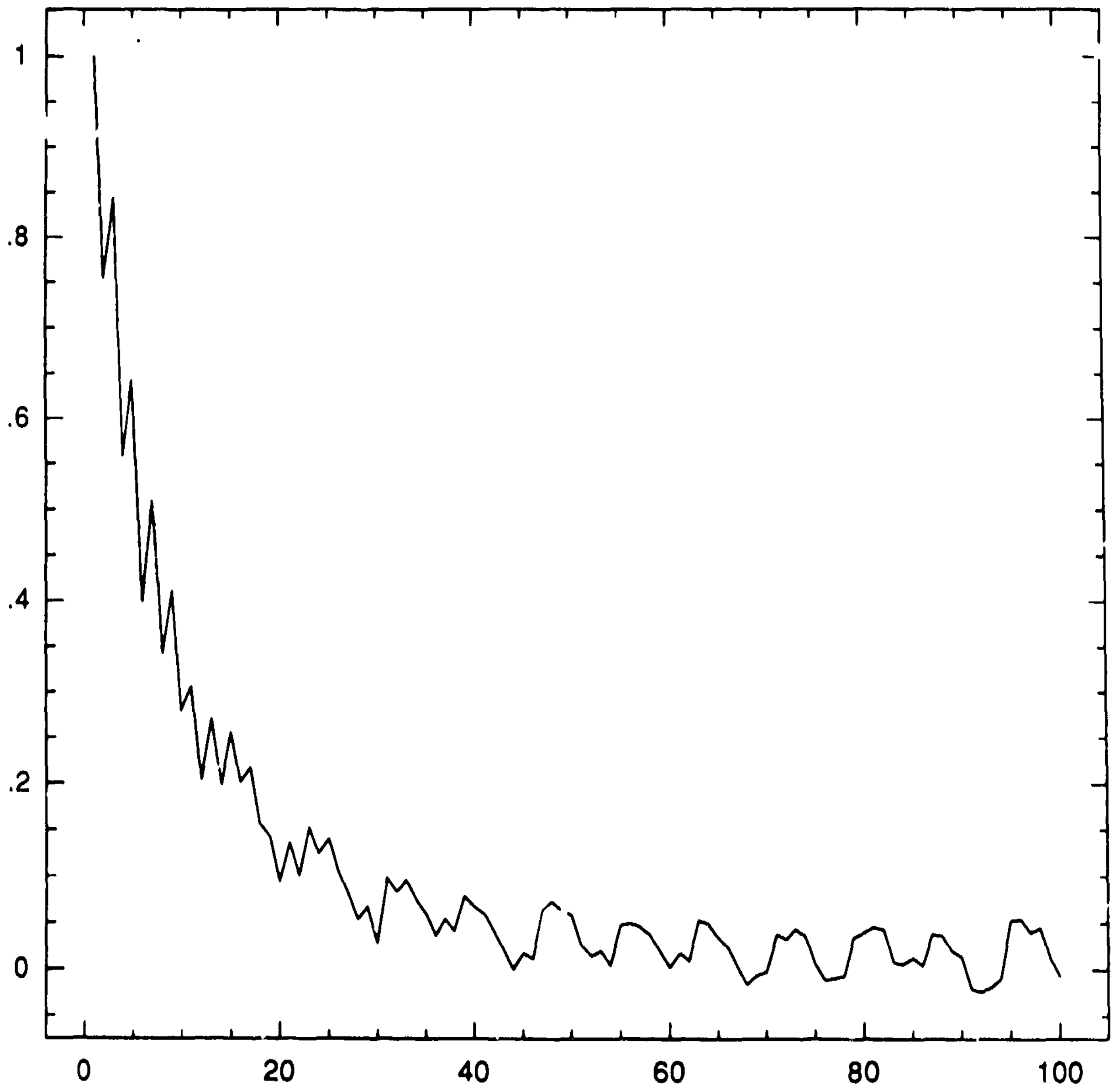

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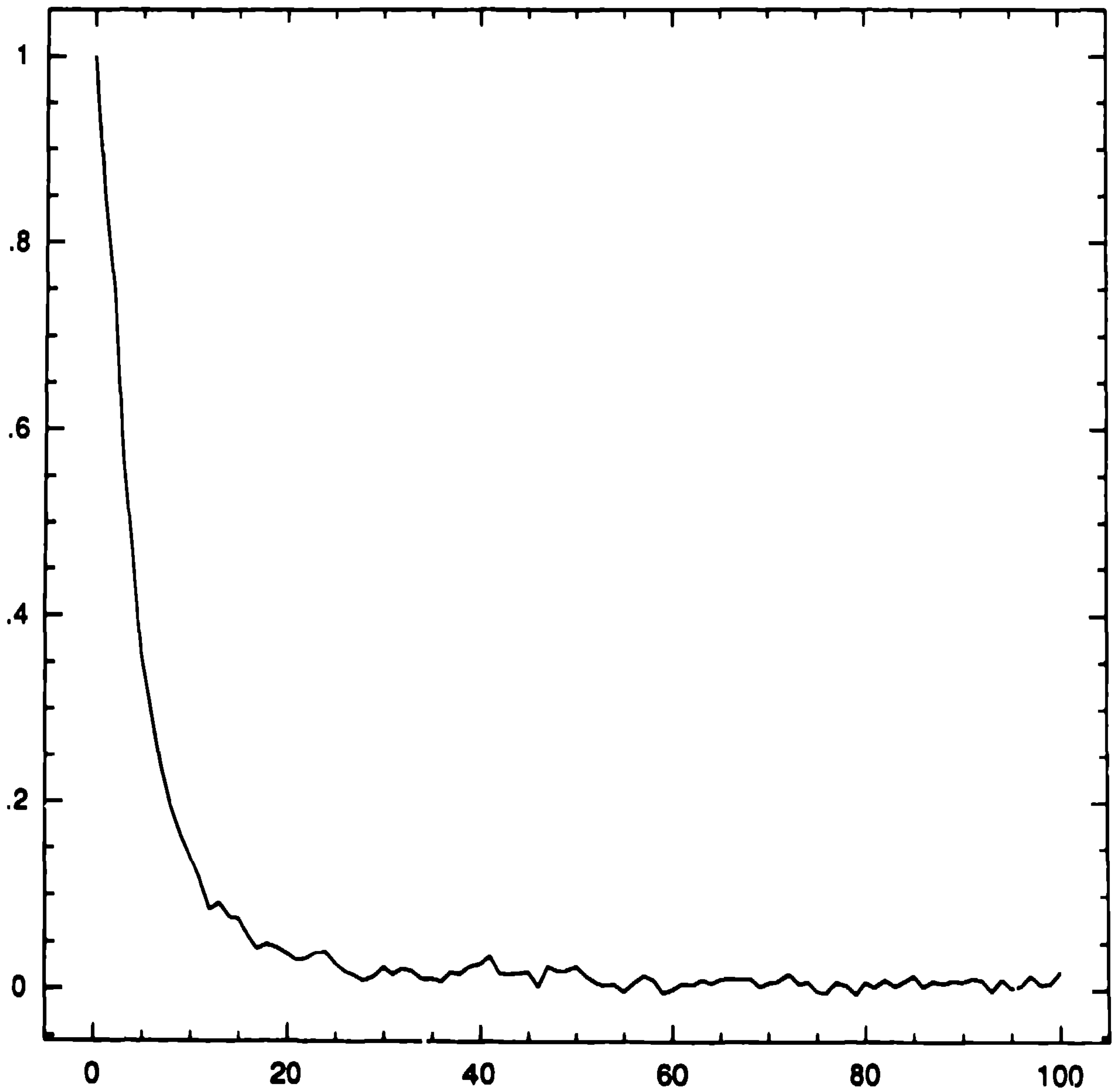

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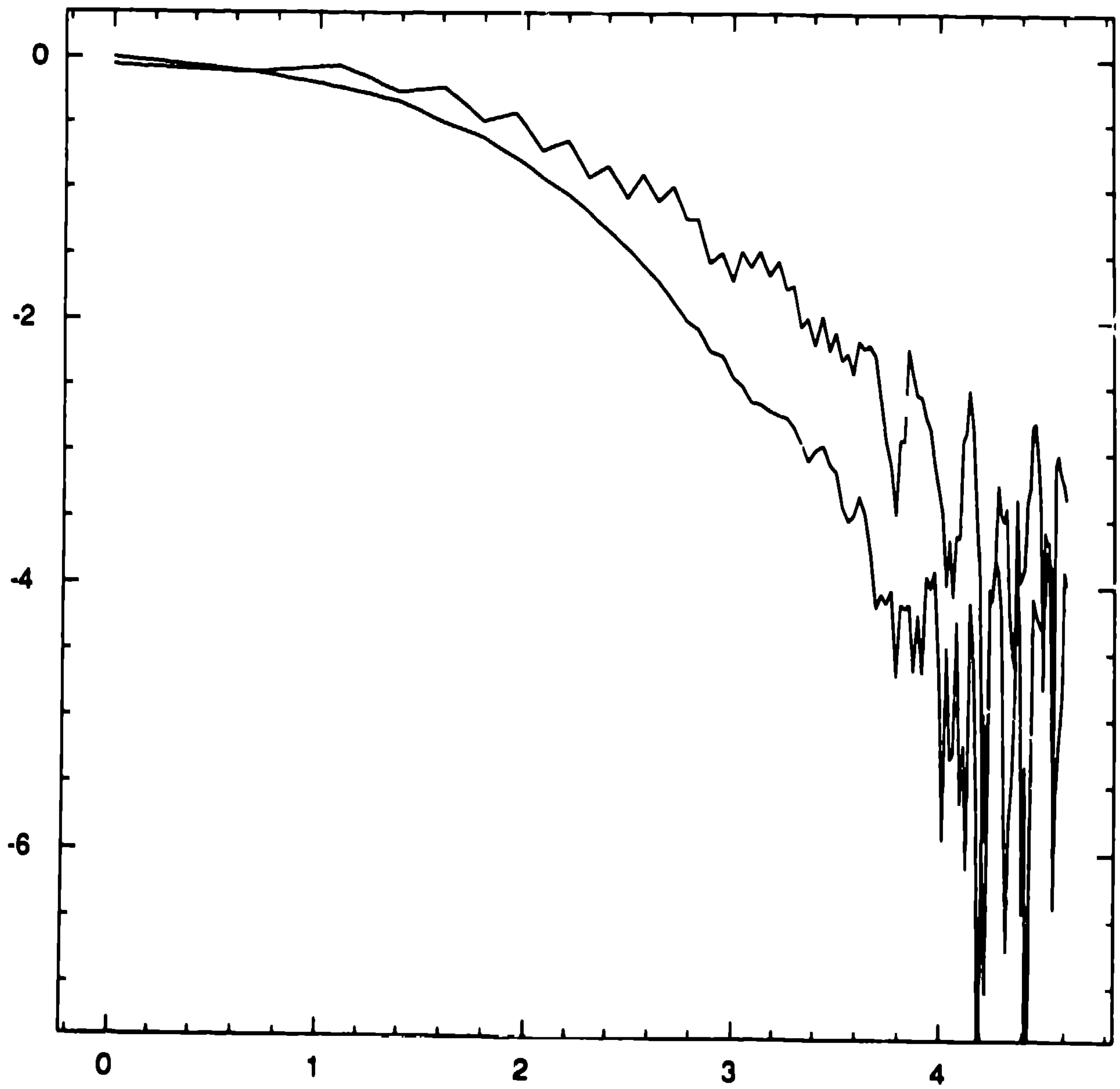

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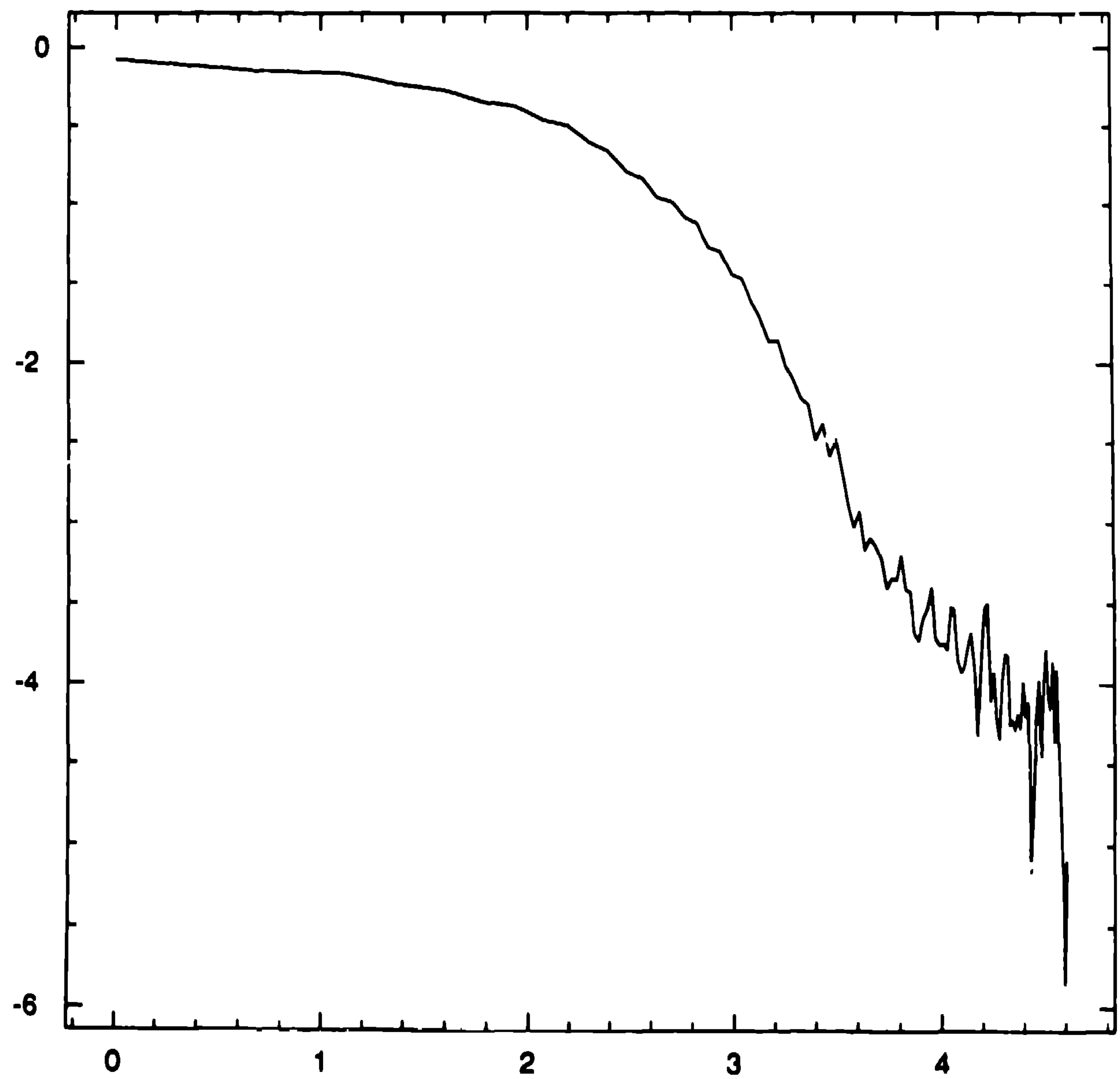

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